



Axial preferred solutions for multiobjective optimal control problems: An application to chemical processes

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Abstract

Detecting the Pareto optimal solutions on the Pareto frontier is one of the most important topics in multiobjective optimal control problems. In real-world control systems, there is needed for the decision-maker to apply their own opinion to find the preferred solution from a large list of Pareto optimal solutions. This paper presents a class of axial preferred solutions for multiobjective optimal control problems in contexts in which partial information on preference weights of objectives is available. These solutions combine both the idea of improvement axis and Pareto optimality with respect to preference information. The axial preferred solution, in addition to taking considerations of decision-makers, provides continuous functions for controlling chemical processes. Numerical results are presented for two problems of chemical processes with two different preferential situations.

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1 Introduction

Multiobjective optimal control problem (MOCP) is concerned with a methodology that can treat complex problems encountered in (bio) chemical engineering, optimal robot paths in mechanical engineering, and optimal rocket trajectories in aerospace engineering, where optimal decisions need to be taken in the presence of trade-offs between several conflicting objectives; see [13, 16, 17].

In single-objective optimal control problem, the determination of the optimum solution among a set of given solutions is clear. However, in the absence of preference information, in multiobjective optimal control, there does not exist a way to determine if a solution is better than other, but, instead, we produce a set of them called the Pareto optimal set [8].

To solve multiobjective optimal control problems, multiobjective optimization methods are used as basic methods. Multiobjective optimization methods depending on how the decision-maker (DM) articulates their preferences divided into four classes: methods that involve a priori articulation of preferences, methods with a posteriori articulation of preferences, methods that require no articulation of preferences are addressed, and interactive methods [6].

In a priori method, preference information is first asked from the DM before running the optimization algorithm, and then a solution best satisfying these preferences is found. In a posteriori method, a representative set of Pareto optimal solutions is first found, and then DM must choose a single solution from a set of solutions. In no preference methods, often the DM cannot concretely define what he or she prefers, but solutions are identified without preference information. In interactive methods, the DM is allowed to search for the most preferred solution iteratively. In each iteration of the interactive method, the DM shows Pareto optimal solutions and describes how the solutions can be improved [5].

Well-known examples of priori methods include the weighted sum method that consists of assigning each objective function a weight coefficient and then optimizing the function obtained by summing up all the objective functions scaled by their weight coefficients that only one solution can be rendered accordingly. With different weights, different Pareto optimal solutions are produced [6]. Though computationally more expensive, this approach gives an idea of the shape of the Pareto front and provides the user with more information about the trade-off among the objectives [22].

Usually it is not economical to generate the entire Pareto surface, due to the high computational cost for function evaluations. Moreover, it may be hard for the DM to choose from a large list. To mitigate these problems, with applying the DM's preferences, it is possible to create situations in which realistic solutions can be obtained that are acceptable to the DM. Since incorporation of the preference information of the DMs and the elicitation of the weights of the objectives are essential problems in multiple objective

optimal control problems, in this paper, we introduce an approach that partly deals with these difficulties. We consider a situation that partial information on the objectives importance is available, that is, the values of these weights are not precisely stated.

There are many methods in literature, in which objective function coefficients or preferential weight coefficients are not exactly specified, but given as intervals or by means of linear relations (see, for instance, [19, 15, 7]). Since these methods focus on the sensitivity of a given solution to feasible changes in the parameters, in this paper, we introduce specific solutions, for multiple objective optimal control problems. These solutions, in addition to taking considerations of DMs, provide continuous functions for controlling chemical processes. When using axial preferred solutions, a weighted sum of the objectives also directs the search for the results. We assume that preferences are originally additive, however, consider an additional element in the form of an improvement axis to better representation. Applying an improvement axis, the different objectives are not treated equally even when the preference information does not differ between them.

The main idea of this paper is to incorporate partial information of the DMs on the preference weights of objectives in order to achieve optimal solutions on the Pareto frontier that are acceptable and realistic for the DM according to their information considerations. In order to achieve this aim, we have to introduce a new concept of solutions, axial preferred solutions, for multiobjective optimal control. These solutions combine both the idea of improvement axis and Pareto optimality with respect to preference information.

The rest of the paper is organized as follows. In Section 2, mathematical formulations of general multiobjective optimal control problem are briefly introduced. Section 3 is devoted to the representation of preference structures and the corresponding definition of efficiency. Also in this section, the idea of improvement axis is described. The axial preferred solutions for multiobjective optimal control problem are introduced in Section 4. In Section 5, two problems are presented with two different preferential situations. Lastly, section 6 outlines the conclusion.

2 Multiobjective optimal control problem

A general multiobjective optimal control problem consists of optimizing a vector of functions is defined as below:

$$Opt (J(x, u) = (J_1(x, u), J_2(x, u), \dots, J_m(x, u)))$$

subject to:

$$\begin{aligned}\dot{x}(t) &= f(x, u, t), \\ g(x, u, t) &\geq 0, \\ \psi(x_0, x_f, t_0, t_f) &\geq 0, \\ t &\in [t_0, t_f].\end{aligned}$$

where J_i are functions of the state variable $x : [t_0, t_f] \rightarrow R^n$, control variable $u \in L^\infty$, and time t . For each individual cost function, let us here consider the following formulation:

$$J_i = \varphi(x_f, t_f) + \int_{t_0}^{t_f} L_i(x, u, t) dt.$$

The objective functions are $J_i : R^{n+2} \times R^p \times [t_0, t_f] \rightarrow R$. The objective vector is subject to a set of dynamic constraints with $f : R^n \times R^p \times [t_0, t_f] \rightarrow R^n$, algebraic constraints $g : R^n \times R^p \times [t_0, t_f] \rightarrow R^s$, and boundary conditions $R^{2n+2} \rightarrow R^q$. The admissible set $\mathcal{P} \subset R^n \times R^p \times [t_0, t_f]$ is defined to be the set of all feasible pairs state and control (x, u) that satisfy in (2-5).

In MOCPs, usually objectives conflict with each other, so it is not easy to have an admissible pair (x^*, u^*) that optimizes all the objectives simultaneously. Therefore, the concept of Pareto optimality is used. The concept of optimality in a single objective is not directly applicable in multiobjective optimization problems. For this reason, a classification of the solutions is introduced in terms of Pareto optimality, according to the following definitions (see [23, 18]) in terms of minimization of objective functions:

Definition 1. It is said that a pair $(x^*, u^*) \in \mathcal{P}$ dominates another pair $(x, u) \in \mathcal{P}$ (denoted by $(x^*, u^*) \succ (x, u)$) if the pair (x^*, u^*) is no worse than the pair (x, u) in all objectives and the pair (x^*, u^*) is strictly better than (x, u) in at least one objective. If there is no solution that dominates (x^*, u^*) , then it is nondominated.

Definition 2. A pair $(x^*, u^*) \in \mathcal{P}$ is a Pareto optimal solution of the MOCP if and only if there is no other pair $(x, u) \in \mathcal{P}$ that dominates (x^*, u^*) .

Definition 3. The set of nondominated pairs $(x^*, u^*) \in \mathcal{P}$ such that $\{(x^*, u^*) \in \mathcal{P} | \neg \exists (x, u) \in \mathcal{P} : (x, u) \succ (x^*, u^*)\}$ is said to be a Pareto set. Also, the set of vectors in the objective space that are images of a Pareto set, is said to be a Pareto frontier.

3 Partial preference information and improvement axis

If a unique vector of weights is available, then the preferred solution is obtained. When several decision makings have to solve a MOP, but do not

agree on the weight of objectives, each DM will propose a different vector of weights for objectives. In this case, we have a partial information on the importance of the objectives. The contribution of this paper is not the elicitation of the weights, instead we want to obtain the whole set of weights considered appropriate by the DM. In fact, we consider a situation in which the weights are not exactly specified, but only partial information about importance of objectives is available. Here, the partial information is denoted by $\Omega \subseteq \Delta^{m-1}$, where $\Delta^{m-1} = \{w \in R_+^m \mid \sum_{r=1}^m w^r = 1\}$. In particular, we consider situations in which Ω is a polyhedron and whose extreme points are w^1, w^2, \dots, w^k .

Definition 4. Suppose that $(x^*, u^*), (x, u) \in \mathcal{P}$. Then it is said that a vector $J(x^*, u^*)$ dominates another pair $J(x, u)$ with respect to $\Omega \subseteq \Delta^{m-1}$ (denote this relationship by $J(x^*, u^*) \succ_{\Omega} J(x, u)$) if $w \cdot J(x^*, u^*) < w \cdot J(x, u)$ for all $w \in \Omega$.

Definition 5. Suppose that $(x^*, u^*), (x, u) \in \mathcal{P}$. Then it is said that a vector $J(x^*, u^*)$ weakly dominates another pair $J(x, u)$ with respect to $\Omega \subseteq \Delta^{m-1}$, denoted by $J(x^*, u^*) \succeq_{\Omega} J(x, u)$, if $w \cdot J(x^*, u^*) \leq w \cdot J(x, u)$ for all $w \in \Omega$.

Definition 6. The point $J(x^*, u^*) \in J(\mathcal{P})$ is said to be Ω -nondominated, if there is no $J(x, u) \in J(\mathcal{P})$ such that $J(x, u) \succ_{\Omega} J(x^*, u^*)$. A pair $(x^*, u^*) \in \mathcal{P}$ is an Ω -Pareto optimal if $J(x^*, u^*)$ is Ω -nondominated.

If there is no information about the weight of the objectives, then all the weights will be possible and, as a result, Ω -Pareto optimal reduces to Pareto-optimality. On the other hand, the highest level of information is available, when a unique vector of weight is provided. The more the partial information, the smaller the set of Ω -Pareto optimal solutions. However, there may still be many Pareto optimal solutions, and more criteria are needed in order to identify the preferred solutions. For this purpose, we combine the idea of Ω -Pareto optimality and improvement axis, which provides a direction in which the improvement of the objective value, and then introduce axial preferred solutions to finding most preferred solution. The existence of a direction to reach the Pareto frontier is the idea behind proportional solutions [9]. We define these solutions in the context of multiobjective optimal control problems as follows.

Definition 7. We say that a pair $(x, u) \in \mathcal{P}$ is a proportional solution for MOCP if there is a strictly positive constant $p \in R^m$ such that $J(x^*, u^*) = h^*p$, where $h^* = \min\{h \in R_+ \mid \exists (x, u) \in \mathcal{P}, J(x, u) = hp\}$ and is denoted by $(x^*, u^*) = P(\mathcal{P}, J)$.

Proportional solutions are not necessarily Pareto optimal, and they not only do not incorporate the preference information, but may also produce results that are unacceptable to DMs (when their preferences incorporated).

For this purpose, here we introduce the solutions that incorporate preferential information and use the idea of improvement axis.

4 Axial preferred solutions for multiobjective optimal control problems

In this section, a multiobjective optimal control problem with partial information is denoted by (\mathcal{P}, J, Ω) . To define the axial preferred solutions, we use both the idea of Ω -Pareto optimality and improvement axis. If the partial information contains rules outside the set of the proportional results, then the axial preferred solution will consist of those results that the decision making considers equivalent to a point in the improvement axis with the highest possible level.

Definition 1. We say that a pair $(x, u) \in \mathcal{P}$ is an axial preferred solution for MOCP with partial information if there is an improvement axis $p \in R_+^m$ such that $J(x, u) \succeq_{\Omega} h^*p$, where $h^* = \min\{h \in R_+ \mid \exists (x, u) \in \mathcal{P}, J(x, u) \succeq_{\Omega} hp\}$ and is denoted by $(x^*, u^*) = A(\mathcal{P}, J, \Omega)$.

Theorem 1. The axial preferred solutions are a subset of the Ω -Pareto optimal solutions.

Proof. Let $(x, u) \in A(\mathcal{P}, J, \Omega)$, and suppose on the contrary that the pair (x, u) is not an Ω -Pareto optimal solution, this means that $J(x, u)$ is dominated with respect to Ω . Then, there exists a pair $(\hat{x}, \hat{u}) \in \mathcal{P}$ such that

$$w^r \cdot J(\hat{x}, \hat{u}) < w^r \cdot J(x, u) \leq w^r h^* p \quad \text{for all } r = 1, \dots, m.$$

Since $p \in R_+$, for each $w \in \Omega$, we have $w \cdot p > 0$ and there is small enough $\epsilon > 0$, such that

$$\epsilon w^r \cdot p > w^r (J(\hat{x}, \hat{u}) - h^* p),$$

and so we have

$$w^r (\epsilon + h^*) p > w^r J(\hat{x}, \hat{u}), \quad \text{for all } r = 1, \dots, m,$$

and this contradicts to $h^* = \min\{h \in R_+ \mid \exists (x, u) \in \mathcal{P}, J(x, u) \succeq_{\Omega} hp\}$. \square

The following theorem shows that axial preferred solutions are depend both on the extreme points of the set of information and on the axis.

Theorem 2. Suppose that w^1, w^2, \dots, w^m are the extreme points of the partial information set, and that $p \in R_+^m$ is the improvement axis. Then

$$A(\mathcal{P}, J, \Omega) = \arg \min_{(x, u) \in \mathcal{P}} M_\Omega(J(x, u)),$$

where

$$M_\Omega(J(x, u)) = \max \left\{ \frac{w^1 \cdot J(x, u)}{w^1 \cdot p}, \frac{w^2 \cdot J(x, u)}{w^2 \cdot p}, \dots, \frac{w^m \cdot J(x, u)}{w^m \cdot p} \right\}. \quad (1)$$

Proof. Given the definition of the preference relations, we have

$$\begin{aligned} h^* &= \min\{h \in R_+ \mid \exists (x, u) \in \mathcal{P}, J(x, u) \succeq_\Omega h.p\} \\ &= \min\{h \in R_+ \mid \exists (x, u) \in \mathcal{P}, w^r \cdot J(x, u) \leq w^r \cdot h.p, r = 1, \dots, m\} \\ &= \min\{h \in R_+ \mid \exists (x, u) \in \mathcal{P}, (w^r \cdot J(x, u)) / (w^r \cdot p) \leq h, r = 1, \dots, m\} \\ &= \min\{h \in R_+ \mid \exists (x, u) \in \mathcal{P}, M_\Omega(J(x, u)) = h\}. \end{aligned}$$

□

The following corollary states that results obtained with axial preferred solutions for a multiobjective optimal control problem can be computed by solving a scalar equivalent optimal control problem.

Corollary 1. Suppose that w^1, w^2, \dots, w^m are the extreme points of the partial information set, and that $p \in R_+^m$ is the improvement axis, Then $(x^*, u^*) \in A(\mathcal{P}, J, \Omega)$, if and only if there exists h^* such that (h^*, x^*, u^*) is an optimal solution to the following problem:

$$\begin{aligned} \min \quad & h \\ \text{s.t. :} \quad & w^r \cdot J(x, u) \leq h w^r \cdot p, \quad r = 1, \dots, m, \\ & (x, u) \in \mathcal{P}. \end{aligned} \quad (2)$$

5 Numerical examples

In this section, we illustrate the performance of the proposed method on two numerical example problems, one involving Fed-Batch bioreactor in Section 5.1 and the other, catalyst mixing problem, in a tubular reactor in Section 5.2. It is a common practice to approximate the state and control variables over a partition of the time horizon in optimal control problems, a process referred to as discretization to obtain an approximate solution (see, for instance, [1, 2, 3, 10, 11]). In this section, a discretized version of problems is solved by using the Ipopt [21]. We use the AMPL [4] as an optimization modeling language, which employs the Ipopt as a solver.

5.1 Fed-Batch Bioreactor

The first MOCP is based on the fed-batch lysine fermentation process investigated by Ohno, Nakanishi, and Takamatsu [17]. The aim is to determine an optimal feeding profile and batch length with respect to conflicting yield and productivity objectives as described by Logist et al. [13].

$$\begin{aligned}\frac{dx_1}{dt} &= \left(0.125 \frac{x_2}{x_4}\right) x_1, \\ \frac{dx_2}{dt} &= -\left(\frac{0.125 x_2}{0.135 x_4}\right) x_1 + 2.8u, \\ \frac{dx_3}{dt} &= -\left[384 \left(0.125 \frac{x_2}{x_4}\right)^2 + 134 \left(0.125 \frac{x_2}{x_4}\right)\right] x_1, \\ \frac{dx_4}{dt} &= u.\end{aligned}$$

with the time $t[h]$ as the independent variable. The state variables are $x_1[g]$, the biomass, $x_2[g]$, the substrate, $x_3[g]$, the product (lysine), and $x_4[L]$, the fermenter volume. The control $u[L/h]$ is the volumetric rate of the feed stream, and the initial conditions are specified as

$$[x_1(0), x_2(0), x_3(0), x_4(0)] = [0.1, 14, 0, 5].$$

The goal is to derive a feeding strategy and batch duration that maximize the productivity, that is, the ratio between the product formed and the process duration

$$J_A = \frac{x_3(t_f)}{t_f},$$

while maximizing the yield, that is, the mass of product is added over the mass of substrate during the operation

$$J_B = \frac{x_3(t_f)}{2.8(x_4(t_f) - x_4(0))}.$$

To cast these maximization problems into a minimization framework, the objective functions are defined as the negative productivity and yield that $J_1 = -J_A$ and $J_2 = -J_B$. Note that clearly t_f is free, but it is subject to the constraint $20 \leq t_f \leq 40$. Constraints are also imposed on the fermenter volume, the feed rate, and the amount of substrate to be added, respectively, as follows:

$$\begin{aligned} 5 &\leq x_4(t) \leq 20, \\ 0 &\leq u(t) \leq 2, \\ 20 &\leq 2.8(x_4(t_f) - 5) \leq 42. \end{aligned}$$

The objective functionals, constraints, and the process equations as given in [12] yield the following biobjective optimal control problem.

$$\begin{aligned} \min & \left(-\frac{x_3(t_f)}{t_f}, -\frac{x_3(t_f)}{2.8(x_4(t_f) - x_4(0))} \right), & (3) \\ \text{s.t. :} & \frac{dx_1}{dt} = \left(0.125 \frac{x_2}{x_4} \right) x_1, \\ & \frac{dx_2}{dt} = - \left(\frac{0.125 x_2}{0.135 x_4} \right) x_1 + 2.8u, \\ & \frac{dx_3}{dt} = - \left[384 \left(0.125 \frac{x_2}{x_4} \right)^2 + 134 \left(0.125 \frac{x_2}{x_4} \right) \right] x_1, \\ & \frac{dx_4}{dt} = u, \\ & [x_1(0), x_2(0), x_3(0), x_4(0)] = [0.1, 14, 0, 5], \\ & 20 \leq t_f \leq 40, \quad 5 \leq x_4(t) \leq 20, \\ & 0 \leq u(t) \leq 2, \quad 20 \leq 2.8(x_4(t_f) - 5) \leq 42. \end{aligned}$$

In this problem, suppose that the DM considers the ratio two to one between the objectives $J_1(x, u)$ and $J_2(x, u)$, respectively ($p = (2, 1)$). Here, we consider two situations, in which the preferences information of DMs are different. In the first situation, the preferences of the DM are represented by the set of information $\Omega_1 = \{w \in \Delta^1 | w_1 \geq w_2, 3w_2 \geq w_1\}$. This means that the importance of $J_1(x, u)$ is no less than the importance of $J_2(x, u)$, and no more than three times the importance of $J_2(x, u)$. The extreme points of Ω_1 are $(\frac{1}{2}, \frac{1}{2})$ and $(\frac{3}{4}, \frac{1}{4})$. An alternative interpretation of this set of information in terms of group decision making is as follows: There are two DMs, one of them considers the first objective three times more important than the second objective, while the other one considers both objectives equally important. In the second situation, the set of information is $\Omega_2 = \{w \in \Delta^1 | w_2 \geq w_1, 2w_1 \geq w_2\}$, extreme points of Ω_2 are $(\frac{1}{3}, \frac{1}{3})$ and $(\frac{1}{3}, \frac{2}{3})$, and the interpretation is analogous. We have the optimal control problems (2) and (3) by applying preferential weights and improving the axis. According to Corollary 1, for this problem with the first and second situations, respectively, we have

$$\begin{aligned}
& \min h \\
\text{subject to} & \quad \text{the same constraints as in (1) and} \\
& -\frac{x_3(t_f)}{t_f} - \frac{x_3(t_f)}{2.8(x_4(t_f) - x_4(0))} \leq 3h, \\
& -3\frac{x_3(t_f)}{t_f} - \frac{x_3(t_f)}{2.8(x_4(t_f) - x_4(0))} \leq 7h,
\end{aligned}$$

$$\begin{aligned}
& \min h \\
\text{subject to} & \quad \text{the same constraints as in (1) and} \\
& -\frac{x_3(t_f)}{t_f} - \frac{x_3(t_f)}{2.8(x_4(t_f) - x_4(0))} \leq 3h, \\
& -\frac{x_3(t_f)}{t_f} - \frac{2x_3(t_f)}{2.8(x_4(t_f) - x_4(0))} \leq 4h.
\end{aligned}$$

The optimal solution of problems (2) and (3) are $(J_1^*, J_2^*) = (-17.148, -18.401)$ and $(J_1^*, J_2^*) = (-19.971, -17.062)$, respectively. The optimal control and the optimal state profiles are shown in Figures 1 and 2, respectively. When productivity is preferred, the initial max part is presented in order to stimulate the biomass growth and hence the lysine production. However, when the focus shifts towards yield optimization, more lysine can be produced with the same amount of substrate but at the expense of longer process times.

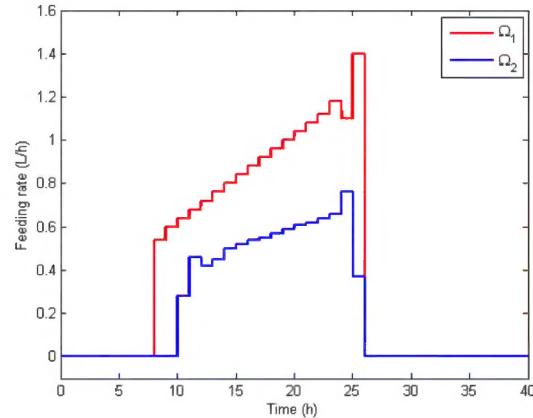


Figure 1: Optimal profile obtained for the control with the first and second situations

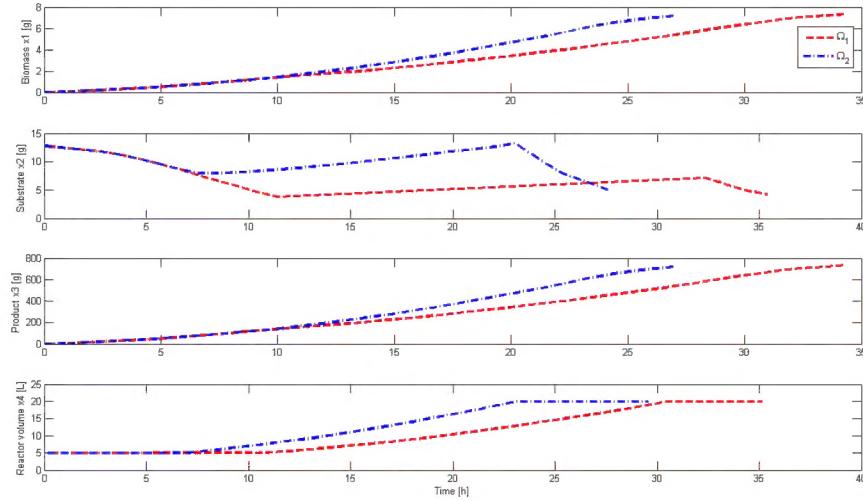


Figure 2: Optimal profiles obtained for the states with the first and second situations

5.2 Catalyst mixing problem in a tubular reactor

The second MOCP considers a steady-state plug flow reactor of fixed length t_f . The reactor is packed with two catalysts. These catalysts are required to stimulate a series of reactions (one reversible and one irreversible $S_1 \leftrightarrow S_2 \rightarrow S_3$). A dynamic model reported by Logist et al. [14] is as follows:

$$\begin{aligned}\frac{dx_1}{dt} &= -u(x_1 - 10x_2), \\ \frac{dx_2}{dt} &= u(x_1 - 10x_2) - (1-u)x_2,\end{aligned}$$

where x_1 and x_2 are the concentrations of S_1 and S_2 and u is the fraction of catalyst A . The original problem, which was introduced by Vassiliadis, Balsa-Canto, and Banga [20], considers the optimal mixing policy of the two catalysts in order to maximize the production at the reactor outlet

$$J_1 = -J_A = (1 - x_1(t_f) - x_2(t_f)),$$

where the reactor has a length t_f equal to 1. To this end the optimal catalyst mixing profiles $u(t)$ and $(1-u(t))$ along the reactor must be determined. The fraction of catalyst A is bounded: $0 \leq u(t) \leq 1$, which directly also bounds the fraction of catalyst B : $0 \leq 1 - u(t) \leq 1$. To introduce a multiobjective nature, the minimization of the amount of the most expensive catalyst (i.e.,

catalyst A) is added as an objective

$$J_2 = J_B = \int_0^t u(t) dt,$$

for given initial conditions

$$x(0) = [1, 0]^T.$$

In this problem, suppose that the DM considers the ratio three to one between the objectives $J_1(x, u)$ and $J_2(x, u)$, respectively ($p = (3, 1)$). As in the previous example, we consider two situations. The preferences of the DM are represented by the set of information $\Omega_1 = \{w \in \Delta^1 | w_1 \geq w_2, 3w_2 \geq w_1\}$ and $\Omega_2 = \{w \in \Delta^1 | w_2 \geq w_1, 2w_1 \geq w_2\}$. By modeling and solving the problem, we obtain $(J_1^*, J_2^*) = (-0.047, 0.216)$ and $(J_1^*, J_2^*) = (-0.015, 0.033)$ for the first and second situations.

Figure 3 shows the optimal profiles for mixing u , concentrations of x_1 and x_2 with the first and second situations. When the focus is put on limiting the use of catalyst A , it is seen that the control consists of one minimum arc, meaning that only catalyst B will be used. However, when the production of species S_3 does play a role, the catalyst profiles exhibit a maximum-singular-minimum type arc structure. The more the focus shifts towards the production of S_3 , the larger the maximum and singular arc become and the higher the values are during the singular interval.

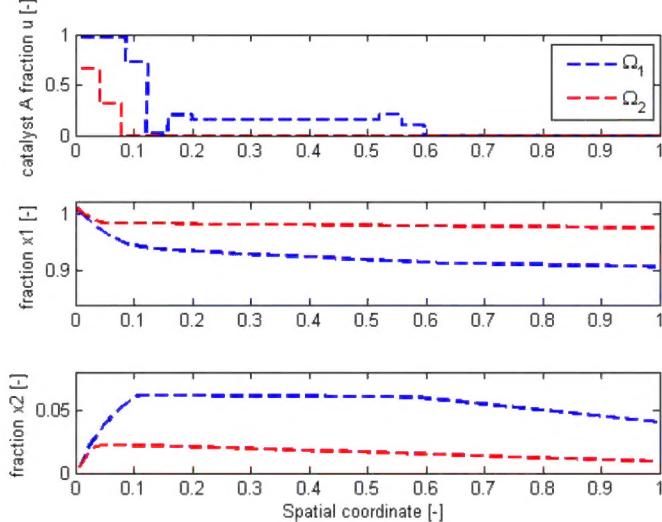


Figure 3: Optimal profiles for mixing u (top), concentrations of x_1 (middle) and x_2 (bottom) with the first and second situations

6 Conclusion

In this paper, we used both the idea of improvement axis and Pareto optimality with respect to preference information and introduced a class of axial preferred solutions for multiobjective optimal control problems in contexts in which partial information on preference weights of objectives is available. It was shown that the axial preferred solutions are a subset of the Pareto optimal solutions. Numerical results were presented for two problems of chemical processes with two different preferential situations. It has been seen that different preferential situations lead to different optimal solutions.

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